Benchmarking of ^{232}Th from ENDF/B-VII.beta3

Andrej Trkov

Jozef Stefan Institute, Ljubljana, Slovenia

20 July 2006

1. Background

The purpose of the benchmarking exercise was to validate the new ^{232}Th and ^{233}U evaluations in the ENDF/B-VII.b3 library. The evaluated nuclear data file for ^{232}Th was developed through the IAEA co-ordinated research project (CRP) on "Evaluated Nuclear Data Files for the Th-U Fuel Cycle"; the ^{233}U evaluation was adopted for the same CRP from the ENDF/B-VII.b3 library after careful review and data intercomparison.

2. Scope

Benchmarks from the ICSBE Handbook that were considered in the analysis are shown in Table 1. The RBMK benchmarks were not analysed because it was felt their sensitivity to thorium data is not very high. Benchmarks in which thorium appears only as an impurity were also excluded.

Table 1.: List of thorium-bearing lattices in ICSBEP.

Ident	Cases		Description
HEU-MET-FAST-068	1	KBR22	KBR22 (U/Th metal, polyethylene)
HEU-MET-INTER-008	1	KBR23	KBR23 (U/Th metal, polyethylene)
IEU-COMP-FAST-002	1	KBR18	KBR18 (90%235UO2+Th metal+36%235UO2)
IEU-COMP-INTER-001	1	KBR19	KBR19 (90%235UO2+Th metal+36%235UO2, polyethylene)
	1	KBR20	KBR20 (90%235UO2+Th metal, polyethylene)
IEU-COMP-THERM-005	1	KBR21	KBR21 (36%235UO2+Th metal, polyethylene)
PU-MET-FAST-008	1	THOR	THOR Pu sphere/Th-reflector
HEU-COMP-THERM-015	1	LWBR SB-1	LWBR SB-1 (93%235UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-5	LWBR SB-5 (93%235UO2+ZrO2, ThO2 blanket)
U233-COMP-THERM-001	1	LWBR SB-2	LWBR SB-2 (97%233UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-2½	LWBR SB-2½ (97%233UO2+ZrO2, no blanket)
	1	LWBR SB-3	LWBR SB-3 (97%233UO2+ZrO2, UO2+ThO2 blanket)
	1	LWBR SB-4	LWBR SB-4 (97%233UO2+ZrO2, UO2+ThO2 blanket)
	1	LWBR SB-6	LWBR SB-6 (97%233UO2+ZrO2, ThO2 blanket)
	1	LWBR SB-7	LWBR SB-7 (97%233UO2+ZrO2, UO2+ThO2 blanket)
LEU-COMP-THERM-060	10	RBMK	RBMK (Th absorbers, cases 19-28)
U233-SOL-THERM-006	1	ORCEF	ORCEF (Th as impurity only)
U233-SOL-THERM-008	1	ORNL	ORNL (Th as impurity only)
U233-SOL-THERM-009	1	ORNL	ORNL (Th as impurity only)
U233-SOL-THERM-012	1	ORCEF	ORCEF (Th as impurity only)
U233-SOL-THERM-013	1	ORCEF	ORCEF (Th as impurity only)

In addition, the benchmark from the SINBAD database on the IPPE leakage spectrum measurement from thorium sphere with a D-T source was considered.

The MCNP5 Monte Carlo code with various data libraries was used in the analysis. The inputs for MCNP5 were taken from the ICSBEP handbook or the SINBAD specifications, but the number of particle histories and the number of batches for k_{eff} determination were increased so that the statistical error in the calculations was negligible compared to experimental uncertainties. Material composition data were also changed where necessary to replace elemental number densities with the corresponding isotopic ones. Sensitivity analysis on the source data libraries was performed. Most of the libraries were available from the MCNPDATA package distribution. The ACE files from ENDF/B-VII.b2 library were obtained from NNDC, Brookhaven. The change in the average number of neutrons per fission at thermal energies for ^{233}U as recommended for ENDF/B-VII.b3 was done locally. Additional libraries and ^{232}Th and ^{233}U files in ACE format were generated at the IAEA and at IJS. It must also be noted that NJOY99 with updates "up125" is insufficient to generate correct ACE files for ^{232}Th, and ^{231,233}Pa, as noted by Marieke Duivestijn. An additional patch is needed to correct the neutron multiplicity flag in the TYR block of the ACE file. The patch was offered to NNDC for consideration. The following libraries were considered in the analysis

ENDF/B-V	The ".50c" series of materials in the RMCCS and RMCCSA files of the MCNPDATA set.
ENDF/B-VI Rel.2	The ".60c" series of materials in the ENDF60 file of the MCNPDATA set.
ENDF/B-VI Rel.4	The ".64c" series of materials in the URESA file of the MCNPDATA set.
ENDF/B-VI Rel.6	The ".66c" series of materials in the ENDF66 files of the MCNPDATA set.
ENDF/B-VI Rel.8	The ".62c" series of materials in the ACTI files of the MCNPDATA set.
ENDF/B-VII.b2,3	The ENDF/B-VII.b2 library generated at NNDC, Brookhaven, with correction for the neutron yield flag in the TYR block. The only change (done locally) for ENDF/B-VII.b3 is the average number of neutrons per fission of ^{233}U.
ADS	Reference library for ADS from the IAEA based on JEFF-3.1 data.

3. Results

The results are presented as the differences between the calculated multiplication factor k_c and the measured one k_m in units of parts per 100 000 (pcm). Separate plots for each set of benchmarks are presented.

KBR benchmarks

In the KBR series of benchmarks, cases 22 and 23 are critical configurations; cases 18 to 21 are k_∞ measurements with progressively softer spectra and are highly sensitive to ^{232}Th data. In Figure 1 the sensitivity of the results on different libraries is presented. The maximum spread in the results with ENDF/B-VI data is around 7000 pcm. The main new feature in ENDF/B-VI Rel.4 compared to Rel.2 is the introduction of probability tables in the unresolved resonance range. KBR-18 and 19 are strongly influenced by the self-shielding in the unresolved resonance range, generally making the results worse. The biggest outliers are KBR-18 and 21 with hardest and softest spectra, respectively. The improvement using ENDF/B-VII.b2 data is significant; the maximum spread of the results is reduced to about 3000 pcm, although the two outliers are still slightly outside the 2σ uncertainty interval. The influence of the new ^{232}Th data alone is shown in Figure 2, confirming that these data are chiefly responsible for the improvement. The KBR benchmarks are strongly influenced by the processing error in generating the ACE files with NJOY99.125. The correction <u>reduces</u> the calculated k_∞ by up to 500 pcm.

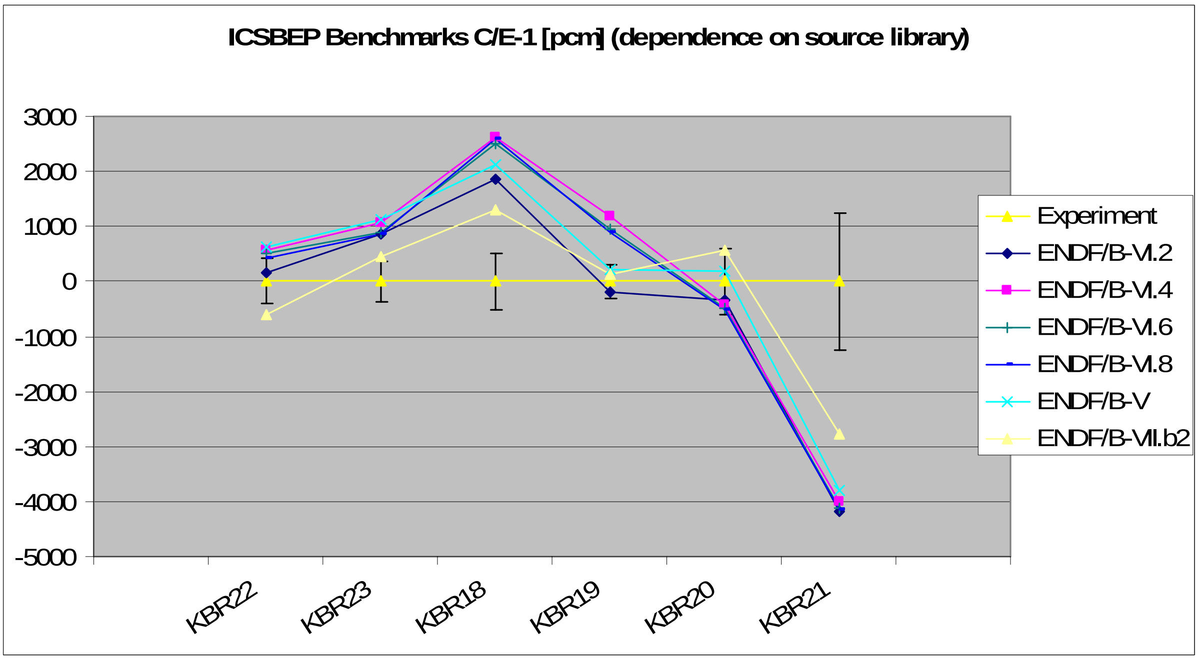

Figure 1.: Results of calculations for the KBR series of benchmarks with different libraries

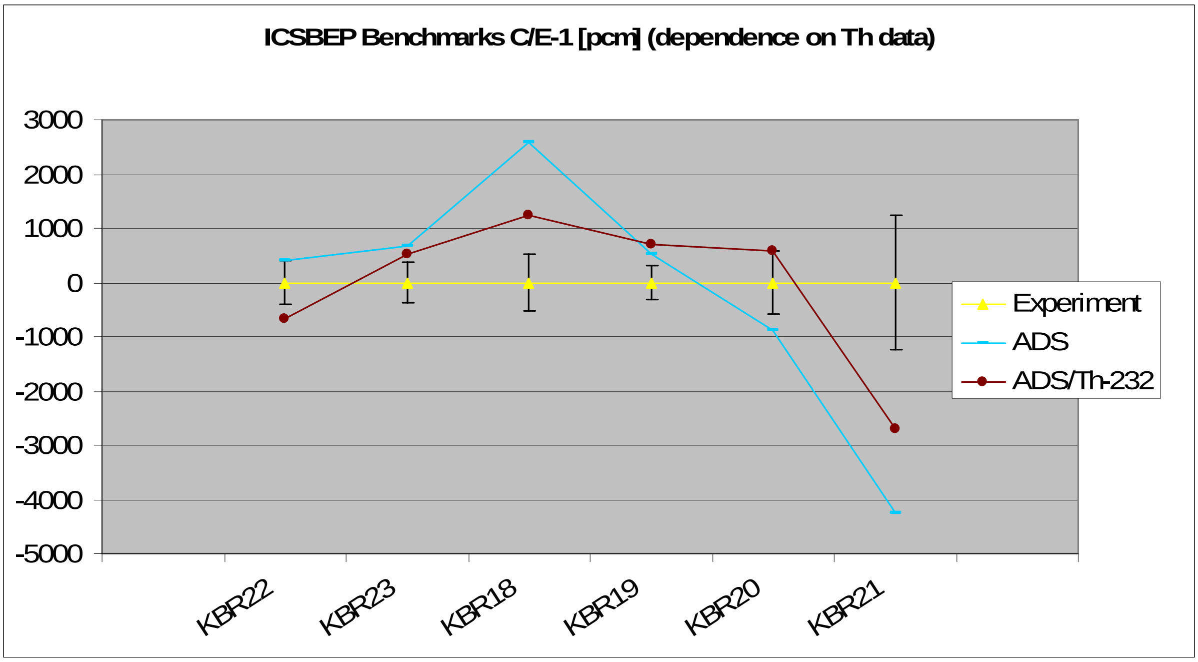

Figure 2.: Sensitivity of the KBR benchmarks on ^{232}Th data

SB-n benchmarks

The SB-n series of benchmarks are thermal lattices with thorium blanket and either ^{235}U (SB-1,5) or ^{233}U (other) fissile component in zirconium matrix fuel. As seen from Figure 3, the change from ENDF/B-V to ENDF/B-VI produced worse results for these benchmarks. The results with the new ENDF/B-VII.b3 data for ^{233}U lie completely within the 1σ uncertainty interval, except for lattice SB-6, which is the only outlier, but still well within the 2σ uncertainty band.

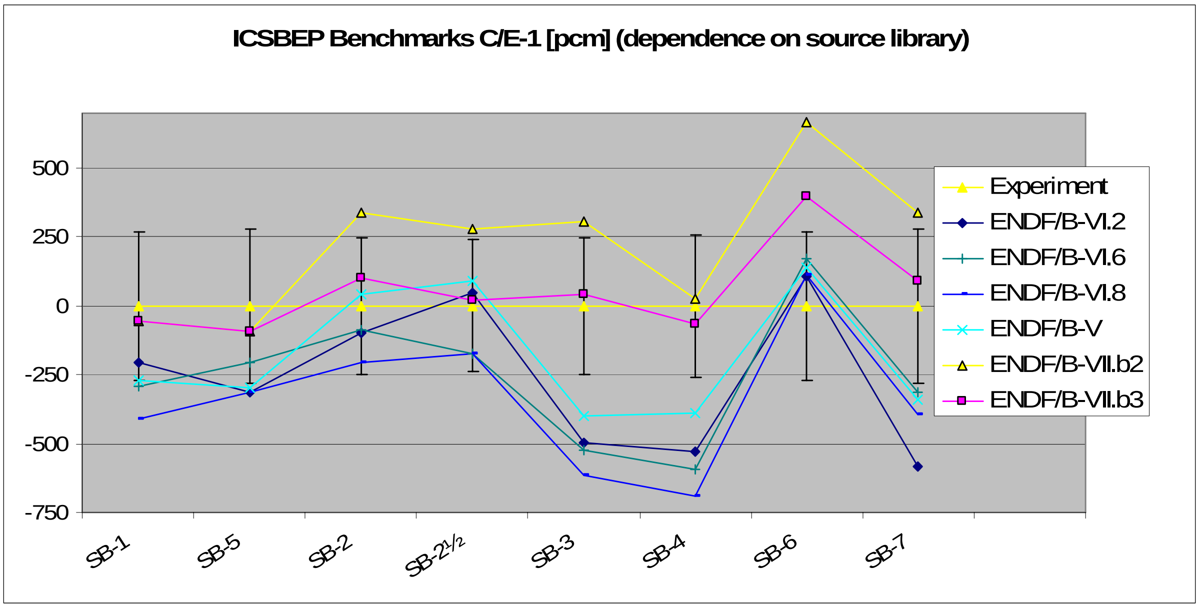

Figure 3.: Results of calculations for the SB-n series of benchmarks with different libraries

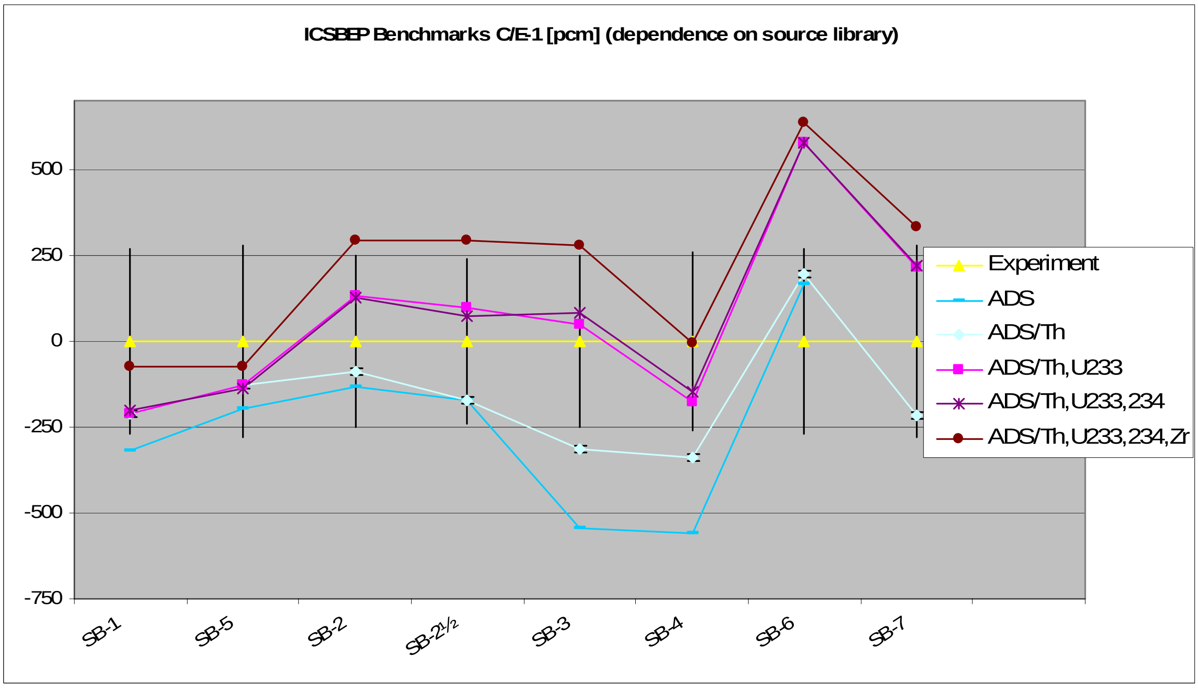

Figure 4.: Sensitivity of the SB-n benchmarks on nuclear data

Sensitivity to nuclear data

Sensitivity to nuclear data of individual nuclides is quite revealing. Starting arbitrarily with the base calculation using ADS library (where ^{232}Th data were taken from ENDF/B-VI.6), the data for ^{232}Th, ^{233}U, ^{234}U and zirconium were replaced with the data from ENDF/B-VII.b2. The results in Figure 4 show strong sensitivity of SB-3 and SB-4 lattices to ^{232}Th data. The new evaluation for ^{232}Th greatly reduces the scattering in the results. The addition of ^{233}U data from ENDF/B-VII.b2 introduces a distinctly positive bias in the lattices that bear ^{233}U, while the impact of ^{234}U is practically negligible.

The data for zirconium, which is the matrix material in the fuel, also produce a positive bias, which together with ^{233}U data cause the over prediction of reactivity. The reduction of the average number of neutrons per fission in ^{233}U of ENDF/B-VII.b3 completely removes the bias, as evident from Figure 3.

Sensitivity to benchmark uncertainties

There is some degree of uncertainty in control blade positions in the benchmark description. Originally the experimenters envisaged control blade position to be determined from the measured bucklings B_z^2 and Equation 1:

$$B_z^2 = \left[\frac{\pi}{H_C + 2\delta} \right]^2 , \qquad \textit{Equation 1}$$

where H_C is the control blade position and δ is the extrapolation distance, determined to be 8 cm from the benchmark case SB-2½, where the control blade position was more accurately known. When analysing the benchmarks this procedure of determining control blade positions was found highly questionable and sensitive to the choice of the measured buckling values, namely:

- *either* buckling averaged over the seed region of the core,
- *or* buckling taken from the centre-most region (Region I) of the core.

The finally adopted value was the average of the two buckling choices, averaged over all cases (except SB-2½) and fixed for all cases, except SB-2½ in which the original experimenters' recommendation could be followed without ambiguities. The final control blade insertion depths were 3.00±0.75 cm for SB-2½ and 3.285±1.695 cm for all other cases. Detailed results in Table 2 give differences from the adopted control blade positions D_i for the two choices of bucklings and the average of the two for each benchmark case. The following observations can be made:

- Values of D_i differ significantly for the two choices of bucklings.
- The average values are close to the adopted and well within the assigned uncertainty, except for case SB-6, where a deeper control blade insertion would be favoured. This benchmark case is precisely the one that seems to be the outlier in Figure 3.

Table 2: Differences in control blade position D_i from adopted, using different assumptions for buckling.

Lattice	D_i(Seed)	D_i(Reg.I)	D_i(Aver.)
SB-1	-0.21	0.20	-0.01
SB-5	0.35	0.33	0.34
SB-2	0.31	-0.12	0.09
SB-2½	0.00	0.00	0.00
SB-3	-0.49	-0.93	-0.71
SB-4	-1.23	-1.27	-1.25
SB-6	2.15	1.79	1.97
SB-7	-0.87	0.01	-0.43

Reliability of control blade positions could be improved and uncertainties reduced by explicit calculations, varying assigned control rod positions and matching the measured axial flux profiles.

Although this information is discussed in the benchmark description, the measured data are not provided.

Thor benchmark

The Thor benchmark is a thorium-reflected plutonium sphere. Interpretation of the results depends strongly on nuclear data for plutonium. Predicted reactivity is 185 pcm below the benchmark value. Considering that independently reported benchmark results for bare plutonium sphere benchmarks with the ENDF/B-VII.b3 library reproduce reactivity well, the calculated result for the Thor benchmark represents a significant improvement compared to the ENDF/B-VI library which was about 500 pcm high. This benchmark is also influenced by the processing error in generating the ACE files. The correction reduces the calculated k_∞ by about 100 pcm.

IPPE sphere leakage current benchmark

Using the SINBAD model the results with the ENDF/B-VII.b3 data agree with the measurement to about 20%. The main difference is in the low-energy tail of the spectrum, where the (n,3n) reaction has the dominant contribution. A reduction of the (n,3n) cross section near threshold would improve the results. This benchmark is strongly influenced by the processing error in generating the ACE files. Without the correction the agreement between measured and calculated spectra at low energies is perfect, but a “hole” in the spectrum is observed between 2 and 6 Mev. The spectra are shown in Figure 5.

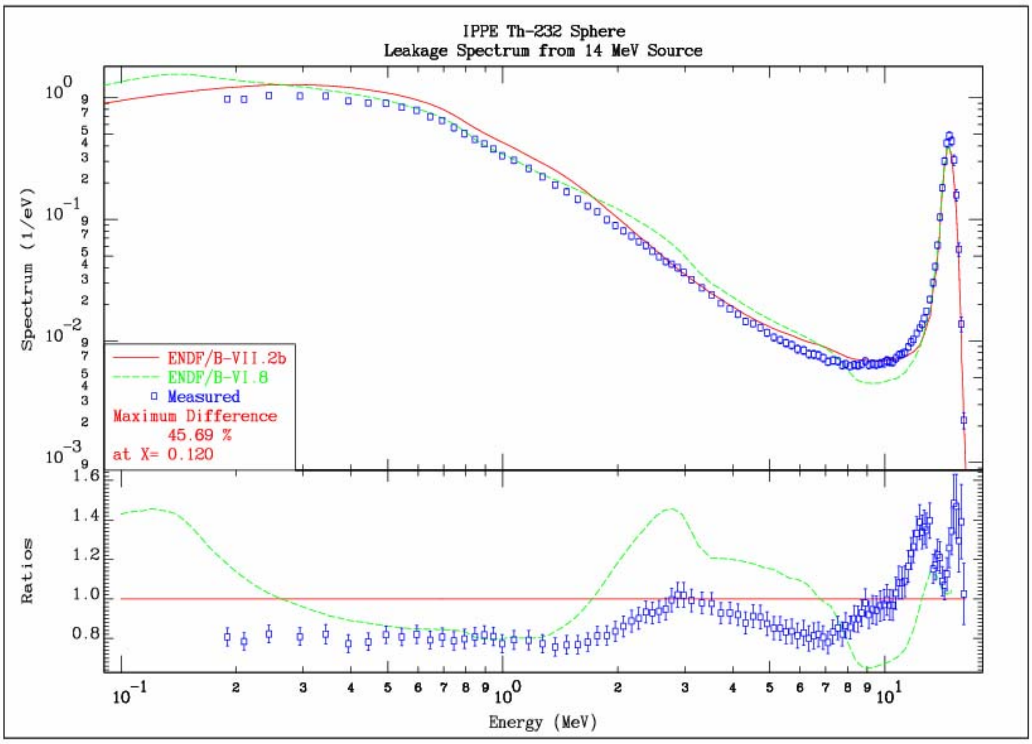

Figure 5.: Leakage spectrum from the IPPE thorium sphere with D-T source.

Apart from the possible cause of the discrepancy between measurement and calculation due to the cross sections, the benchmark model itself is an approximation to the real configuration. It does not model the collimator explicitly. Instead, the benchmark recommendation is to use the source spectrum without the sphere in place to simulate the resolution broadening effects. Unfortunately the available information on the benchmark is insufficient to improve the model.

Conclusions

The results of benchmark calculations are summarised in Table 3. The KBR benchmarks indicate a clear improvement when the ENDF/B-VII.b2 data are used, although the discrepancies for the lattices with the hardest and the softest spectrum still slightly exceed the 2σ level; experimental uncertainties are large and a possible problem with the measurement or its interpretation cannot be ruled out. The swing to over predict reactivity with ENDF/B-VII.b2 data in the SB-n benchmarks with ^{233}U fuel seems to originate from the ^{233}U data and not from thorium. The bias is practically eliminated with the reduction of the average neutrons per fission in ^{233}U for ENDF/B-VII.b3. Further improvement and reduction of experimental uncertainties seems possible by refining the procedures for determining the control blade positions in the SB-n benchmark cases. The results for the Thor benchmark are slightly low but satisfactory. The IPPE thorium sphere leakage benchmark tests the data at higher energies. Before assigning the discrepancies between measurements and calculations to the data, the effect of an explicit model of the collimator should be investigated.

Table 3.: Differences between calculated and measured multiplication factor in units 10^5(C/E-1).

Case	k-eff	Unc. [pcm]	ENDF/B-V	ENDF/B-VI.8	ENDF/B-VII.b3
THOR	1.00000	60	620	567	-187
KBR22	1.00010	410	630	434	-602
KBR23	1.00080	360	1119	874	453
KBR18	0.96900	516	2126	2593	1286
KBR19	0.98000	306	214	882	118
KBR20	1.01400	592	178	-527	574
KBR21	0.96400	1245	-3807	-4154	-2762
SB-1	1.00060	270	-270	-410	-53
SB-5	1.00150	280	-300	-316	-93
SB-2	1.00150	250	40	-204	123
SB-2½	1.00000	240	90	-175	23
SB-3	1.00070	250	-400	-618	40
SB-4	1.00150	260	-389	-690	-65
SB-6	0.99950	270	140	111	400
SB-7	1.00040	280	-340	-397	92